

Landauer formula for phonon heat conduction: relation between energy transmittance and transmission coefficient

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Abstract

The heat current across a quantum harmonic system connected to reservoirs at different temperatures is given by the Landauer formula, in terms of an integral over phonon frequencies ω , of the energy transmittance $\mathcal{T}(\omega)$. There are several different ways to derive this formula, for example using the Keldysh approach or the Langevin equation approach. The energy transmittance $\mathcal{T}(\omega)$ is usually expressed in terms of nonequilibrium phonon Green's function and it is expected that it is related to the transmission coefficient $\tau(\omega)$ of plane waves across the system. In this paper, for a one-dimensional set-up of a finite harmonic chain connected to reservoirs which are also semi-infinite harmonic chains, we present a simple and direct demonstration of the relation between $\mathcal{T}(\omega)$ and $\tau(\omega)$. Our approach is easily extendable to the case where both system and reservoirs are in higher dimensions and have arbitrary geometries, in which case the meaning of τ and its relation to \mathcal{T} are more non-trivial.

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I. INTRODUCTION

The Landauer formula gives an exact expression for the current (energy and/or particle) in “non-interacting” quantum systems coupled to reservoirs kept at different temperatures (and/or different chemical potentials). By “non-interacting” one refers to systems described by quadratic Hamiltonians. It thus includes harmonic crystals where one considers energy transport by phonons, and tight-binding Hamiltonians where there is transport of both charge and energy by electrons. The formula for phonon heat current across a harmonic crystal connected to heat baths at temperatures T_L, T_R is given by

$$J = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \hbar\omega \, \mathcal{T}(\omega) [f(\omega, T_L) - f(\omega, T_R)] , \quad (1)$$

where the quantity $\mathcal{T}(\omega)$, which we shall refer to as the energy transmittance, can be expressed in terms of appropriate “nonequilibrium” phonon’s Green’s functions and $f(\omega, T) = 1/(e^{\hbar\omega/k_B T} - 1)$ is the thermal phonon distribution function. This Landauer formula for phononic heat current has been derived rigorously using the quantum Langevin equation approach [1, 2] as well as the nonequilibrium Green’s function (NEGF) approach [3, 4].

Landauer’s original idea was to think of conductance in terms of transmission or scattering of plane waves and for the case where the reservoirs or “leads” are one dimensional, it is expected that $\mathcal{T}(\omega)$ is related to the transmission coefficient $\tau(\omega)$ of plane waves [5]. For the case of electron transmission, $\mathcal{T}(\omega)$ can again be expressed in terms of nonequilibrium Green’s functions [6] and the relation to the transmission coefficient was directly demonstrated through the work of Todorov *et al* using scattering theory [7]. For the case of phonons we are not aware of an explicit proof of this relation and that is the main objective of this paper. Here we consider a general one-dimensional finite harmonic chain coupled to reservoirs which are themselves semi-infinite ordered harmonic chains and give a fully quantum-mechanical derivation of the relation between \mathcal{T} and τ and show how the NEGF current formula can be obtained from the transmission coefficient.

In our derivation we first note that in the NEGF approach the energy transmission \mathcal{T} is expressed in terms of a Green’s function. This Green’s function can be expressed explicitly in terms of a product of 2×2 matrices. On the other hand the transmission coefficient can be computed by constructing appropriate scattering states and this can be done in two ways — (i) a direct solution of the discrete wave equation which again gives τ expressed in the form of a product of matrices or (ii) by using the Lippmann-Schwinger scattering

theory to evolve reservoir normal modes and this gives τ directly in terms of the Green's function. From the forms of these expressions we directly obtain the required relations. We note that for the case where the reservoirs are not one-dimensional chains, but have arbitrary geometries [8–10], the NEGF expression for $\mathcal{T}(\omega)$ still has the same form but it is not clear as to how one should compute τ and how exactly it is related to \mathcal{T} . In this case the approach using Lippmann-Schwinger scattering theory can still be used to arrive at the required relation. A model similar to ours was studied recently by Zhang *et al* [11] in the context of interfacial thermal transport in atomic junctions and the relation between the NEGF formula for energy transmittance and the transmission coefficient was established numerically and also exactly for the special case of a single interface.

The plan of the paper is as follows. In sec. II we first define the model and state some general results for the heat current given by the formalism of nonequilibrium Green's functions. We then give an explicit expression for the form of the Green's function appearing in the energy transmission formula. In sec. III we consider the transmission of plane waves across the system and, using two different approaches, obtain the form of the transmission coefficient. The transmission coefficient can also be expressed in terms of the same nonequilibrium Green's function and using this we write the relation between it and $\mathcal{T}(\omega)$. This relation is then used in sec. IV to derive the Landauer formula for heat current. Finally we discuss our results in sec. V.

II. ONE-DIMENSIONAL CHAIN CONNECTED TO ONE-DIMENSIONAL BATHS

Consider the set-up in Fig. (1) where a one-dimensional (1D) harmonic chain with arbitrary spring constants and masses is connected to leads which are themselves ordered harmonic chains. Special cases of this setup have been discussed earlier by various authors [11–16] in the context of heat conduction. Let us assume that the system has N Cartesian positional degrees of freedom $\{x_l\}$, $l = 1, 2, \dots, N$ with corresponding momenta $\{p_l\}$. These satisfy the usual commutation relations $[x_l, p_m] = i\hbar\delta_{l,m}$ and $[x_l, x_m] = [p_l, p_m] = 0$. Similarly the left reservoir degrees of freedom are denoted by $\{x_\alpha, p_\alpha\}$, $\alpha = 1, \dots, N_L$ and the right reservoirs by $\{x_{\alpha'}, p_{\alpha'}\}$, $\alpha' = 1, \dots, N_R$. We consider our system plus reservoir to be described by the

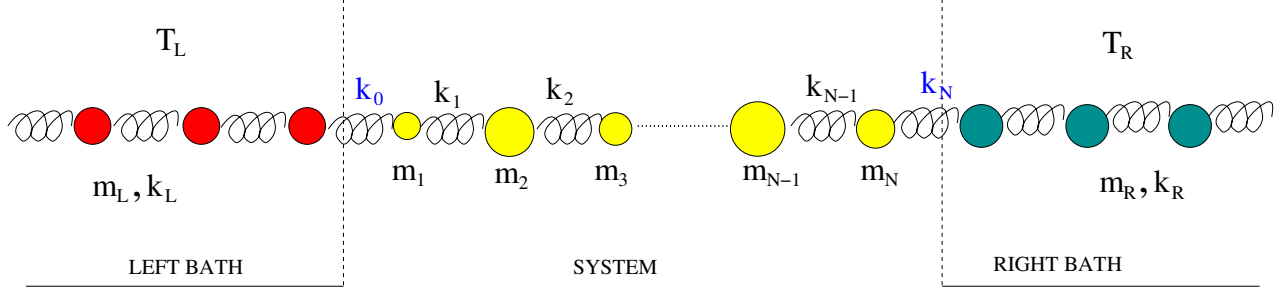


FIG. 1: Schematic of the set-up considered in the paper. The system consists of a harmonic chain of N particles for which both the particle masses and the inter-particle spring constants take arbitrary values. The system is sandwiched between two reservoirs which are ordered 1D harmonic chains with different mass densities and elasticities. The coupling constant between left reservoir and system is k_0 and between right reservoir and system is k_N .

full Hamiltonian

$$\begin{aligned}
\mathcal{H} = & \sum_{l=1}^N \frac{p_l^2}{2m_l} + \sum_{l=1}^{N-1} \frac{k_l(x_l - x_{l+1})^2}{2} \\
& + \sum_{\alpha=1}^{N_L} \frac{p_\alpha^2}{2m_L} + \sum_{\alpha=1}^{N_L} \frac{k_L(x_\alpha - x_{\alpha+1})^2}{2} + \frac{k_0(x_{\alpha=1} - x_1)^2}{2} \\
& + \sum_{\alpha'=1}^{N_R} \frac{p_{\alpha'}^2}{2m_R} + \sum_{\alpha'=1}^{N_R} \frac{k_R(x_{\alpha'} - x_{\alpha'+1})^2}{2} + \frac{k_N(x_{\alpha'=1} - x_N)^2}{2} , \tag{2}
\end{aligned}$$

where we assume $x_{\alpha=N_L+1} = x_{\alpha'=N_R+1} = 0$. The system masses $\{m_l\}$ and spring constants $\{k_l\}$ are assumed to be arbitrary. The left (right) reservoir particle masses are all taken to be m_L (m_R) and the inter-particle spring constants are taken to be k_L (k_R). To ensure a unique steady state We will always assume that the reservoirs are chosen to have sufficiently broad bandwidths compared to the spectrum of the system [1, 18]. The above Hamiltonian can be written in the canonical form:

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_{LS} + \mathcal{H}_{RS} , \tag{3}$$

where

$$\begin{aligned}
\mathcal{H}_S &= \sum_{l=1}^N \frac{p_l^2}{2m_l} + \sum_{l=1}^{N-1} \frac{k_l(x_l - x_{l+1})^2}{2} + \frac{k_0 x_1^2}{2} + \frac{k_N x_N^2}{2}, \\
\mathcal{H}_L &= \sum_{\alpha=1}^{N_L} \frac{p_\alpha^2}{2m_L} + \frac{k_L(x_\alpha - x_{\alpha+1})^2}{2} + \frac{k_0 x_{\alpha=1}^2}{2}, \\
\mathcal{H}_R &= \sum_{\alpha'=1}^{N_R} \frac{p_{\alpha'}^2}{2m_R} + \frac{k_R(x_{\alpha'} - x_{\alpha'+1})^2}{2} + \frac{k_N x_{\alpha'=1}^2}{2}, \\
\mathcal{H}_{LS} &= -k_0 x_{\alpha=1} x_1, \quad \mathcal{H}_{RS} = -k_N x_{\alpha'=1} x_N.
\end{aligned} \tag{4}$$

Using the vector notation $X_S^T = (x_1, x_2, \dots, x_N)$, $P_S^T = (p_1, p_2, \dots, p_N)$ and similarly X_L, X_R, P_L, P_R , the different parts in the above Hamiltonian can be written as

$$\begin{aligned}
\mathcal{H}_S &= \frac{1}{2} P_S^T \mathbf{M}_S^{-1} P_S + \frac{1}{2} X_S^T \mathbf{K}_S X_S, \\
\mathcal{H}_L &= \frac{1}{2} P_L^T \mathbf{M}_L^{-1} P_L + \frac{1}{2} X_L^T \mathbf{K}_L X_L, \\
\mathcal{H}_R &= \frac{1}{2} P_R^T \mathbf{M}_R^{-1} P_R + \frac{1}{2} X_R^T \mathbf{K}_R X_R, \\
\mathcal{H}_{LS} &= X_S^T \mathbf{K}_{SL} X_L, \quad \mathcal{H}_{RS} = X_S^T \mathbf{K}_{SR} X_R,
\end{aligned}$$

where $\mathbf{M}_S, \mathbf{M}_L, \mathbf{M}_R$ and $\mathbf{K}_S, \mathbf{K}_L, \mathbf{K}_R$ denote respectively the mass matrix and the force-constant matrix of the system, left reservoir and right reservoir, while \mathbf{K}_{SL} and \mathbf{K}_{SR} denote the linear coupling coefficients between the two reservoirs and the system. In our case \mathbf{K}_{SL} is a $N \times N_L$ matrix whose only non-zero element is $[\mathbf{K}_{SL}]_{1,1} = k_0$, while \mathbf{K}_{SR} is a $N \times N_R$ matrix whose only non-zero element is $[\mathbf{K}_{SR}]_{N,1} = k_N$.

Expression for steady state heat current: We now consider the situation where at some distant past time ($t < t_0$) the two reservoirs are uncoupled from the system and are separately in equilibrium (and described by canonical distributions) at temperatures T_L and T_R respectively. At time t_0 we start evolving the system plus reservoirs with the full Hamiltonian in Eq. (3). Eventually we set the reservoir sizes $N_L, N_R \rightarrow \infty$ and $t_0 \rightarrow -\infty$. The system reaches a nonequilibrium steady state at finite t . Note that we have included terms involving the coupling coefficients k_0, k_N in the isolated reservoir Hamiltonians. As has been discussed using various approaches [1, 3, 4], the steady state current can be expressed using the following phonon Green's function:

$$\mathbf{G}^\pm = \frac{1}{-\mathbf{M}_S \omega^2 + \mathbf{K}_S - \Sigma_L^\pm - \Sigma_R^\pm}, \tag{5}$$

where the self-energies $\Sigma_L^\pm, \Sigma_R^\pm$ can be expressed in terms of the isolated reservoir Green functions $\mathbf{g}_L^\pm(\omega) = [-\mathbf{M}_L(\omega \pm i\epsilon)^2 + \mathbf{K}_L]^{-1}$, $\mathbf{g}_R^\pm(\omega) = [-\mathbf{M}_R(\omega \pm i\epsilon)^2 + \mathbf{K}_R]^{-1}$ and the coupling matrices $\mathbf{K}_{SL}, \mathbf{K}_{SR}$. The self energies are given by $\Sigma_L^\pm(\omega) = \mathbf{K}_{SL} \mathbf{g}_L^\pm(\omega) \mathbf{K}_{SL}^T$, $\Sigma_R^\pm(\omega) = \mathbf{K}_{SR} \mathbf{g}_R^\pm(\omega) \mathbf{K}_{SR}^T$. Defining $\Gamma_L(\omega) = \text{Im}[\Sigma_L^+]$, $\Gamma_R(\omega) = \text{Im}[\Sigma_R^+]$, we find [1, 3, 4] that the steady state current is given by the formula in Eq. (1) with

$$\mathcal{T}(\omega) = 4\text{Tr}[\mathbf{G}_+(\omega)\Gamma_L(\omega)\mathbf{G}_-(\omega)\Gamma_R(\omega)] . \quad (6)$$

For our one-dimensional system, we note that $\mathbf{G}^\pm, \Sigma_L^\pm, \Sigma_R^\pm$ are all $N \times N$ matrices. The only non-zero elements of Σ_L^\pm and Σ_R^\pm are respectively $[\Sigma_L^\pm]_{1,1} = k_0^2[\mathbf{g}_L^\pm]_{1,1} =: \Sigma_L^\pm$ and $[\Sigma_R^\pm]_{N,N} = k_N^2[\mathbf{g}_R^\pm]_{1,1} =: \Sigma_R^\pm$. Let us define $\Gamma_L = \text{Im}[\Sigma_L^+]$, $\Gamma_R = \text{Im}[\Sigma_R^+]$. Hence the expression of \mathcal{T} reduces to:

$$\mathcal{T} = 4\Gamma_L\Gamma_R\mathbf{G}_{1,N}^+\mathbf{G}_{N,1}^- = 4\Gamma_L\Gamma_R|\mathbf{G}_{1,N}^+|^2 , \quad (7)$$

with the matrix $\mathbf{G}^+ = \mathbf{Z}^{-1}$, where $\mathbf{Z} = -\mathbf{M}_S\omega^2 + \mathbf{K}_S - \Sigma_L^+ - \Sigma_R^+$ is a tri-diagonal matrix. The bandwidth of the two baths are different ($2\sqrt{k_L/m_L}$ and $2\sqrt{k_R/m_R}$ for the left and right baths respectively), so the conduction of heat across the system will have contribution only from the overlapping part of the bandwidths.

Explicit forms for $\mathbf{G}_{1,N}^+, \Gamma_L, \Gamma_R$: Using methods described in [17] we now show that the Green's function element occuring in Eq. (7) can be expressed in terms of a product of 2×2 matrices. We also obtain the explicit forms of Γ_L, Γ_R for our particular model. The matrix \mathbf{Z} has the form

$$\mathbf{Z}(\omega) = \begin{bmatrix} a_1 - \Sigma_L^+(\omega) & -k_1 & \cdots & 0 & 0 & 0 \\ -k_1 & a_2 & -k_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -k_{N-2} & a_{N-1} & -k_{N-1} \\ 0 & 0 & 0 & \cdots & -k_{N-1} & a_N - \Sigma_R^+(\omega) \end{bmatrix} , \quad (8)$$

where $a_l = k_l + k_{l-1} - m_l\omega^2$, $l = 1, \dots, N$.

Taking the inverse of this matrix, we get

$$\mathbf{G}_{1,N}^+ = \frac{\prod_{l=1}^{N-1} k_l}{\Delta_{1,N}} , \quad (9)$$

where $\Delta_{1,N}$ is defined as the determinant of the matrix $\mathbf{Z}(\omega)$. Let us also define $D_{l,j}$ as the determinant of the sub-matrix starting with the l -th row and column and ending with the j -th row and column of the matrix $-\mathbf{M}_S\omega^2 + \mathbf{K}_S$. From the tri-diagonal form of the matrices, it is easily shown that

$$\begin{aligned}\Delta_{1,N} &= (a_1 - \Sigma_L^+) [(a_N - \Sigma_R^+) D_{2,N-1} - k_{N-1} D_{2,N-2}] - k_1 [(a_N - \Sigma_R^+) D_{3,N-1} - k_{N-1} D_{3,N-2}] \\ &= D_{1,N} - \Sigma_R^+ D_{1,N-1} - \Sigma_L^+ D_{2,N} + \Sigma_L^+ \Sigma_R^+ D_{2,N-1} \\ &= \begin{bmatrix} 1 & -\Sigma_L^+ \end{bmatrix} \begin{bmatrix} D_{1,N} & -D_{1,N-1} \\ D_{2,N} & -D_{2,N-1} \end{bmatrix} \begin{bmatrix} 1 \\ \Sigma_R^+ \end{bmatrix}.\end{aligned}\quad (10)$$

The elements $D_{l,j}$ satisfy the recursion relation $D_{l,N} = a_l D_{l+1,N} - k_l^2 D_{l+2,N}$ for $l = 1, \dots, N-2$, and $D_{l,N-1} = a_l D_{l+1,N-1} - k_l^2 D_{l+2,N-1}$ for $l = 1, \dots, N-3$. In matrix form these give

$$\begin{bmatrix} D_{l,N} & -D_{l,N-1} \\ D_{l+1,N} & -D_{l+1,N-1} \end{bmatrix} = k_l \begin{bmatrix} a_l/k_l & -k_l \\ 1/k_l & 0 \end{bmatrix} \begin{bmatrix} D_{l+1,N} & -D_{l+1,N-1} \\ D_{l+2,N} & -D_{l+2,N-1} \end{bmatrix}, \quad (11)$$

which holds for $l = 1, \dots, N-3$. Using these relations and further defining $D_{N+1,N} = D_{N,N-1} = 1$, $D_{N+2,N} = D_{N+1,N-1} = 0$, we arrive at the result

$$\begin{bmatrix} D_{1,N} & -D_{1,N-1} \\ D_{2,N} & -D_{2,N-1} \end{bmatrix} = \prod_{l=1}^N k_l \hat{T} \begin{bmatrix} 1 & 0 \\ 0 & 1/k_N^2 \end{bmatrix}, \quad (12)$$

$$\text{where } \hat{T} \equiv \prod_{l=1}^N \hat{T}_l, \quad \hat{T}_l = \begin{bmatrix} a_l/k_l & -k_l \\ 1/k_l & 0 \end{bmatrix}. \quad (13)$$

Hence using Eqs. (10,12,13) we get

$$\Delta_{1,N} = \left(\prod_{l=1}^N k_l \right) \begin{bmatrix} 1 & -\Sigma_L^+ \end{bmatrix} \hat{T} \begin{bmatrix} 1 & 0 \\ 0 & 1/k_N^2 \end{bmatrix} \begin{bmatrix} 1 \\ \Sigma_R^+ \end{bmatrix}. \quad (14)$$

We next find the explicit forms of Σ_L^+ , Σ_R^+ , for which we need to evaluate the reservoir Green's function elements $[\mathbf{g}_L^+]_{1,1}$ and $[\mathbf{g}_R^+]_{1,1}$. Consider the left reservoir. For the case $k_0 = k_L$, it is simple to find all normal modes and hence compute the Green's function corresponding to the force matrix $\mathbf{K}_L = \mathbf{K}_L^0$ (say). One gets

$$\begin{aligned}\mathbf{g}_L^{0+} &= \frac{1}{-\mathbf{M}_L (\omega + i\epsilon)^2 + \mathbf{K}_L^0} \\ \text{Hence } [\mathbf{g}_L^{0+}]_{l,m} &= \frac{2}{m_L \pi} \int_0^\pi dq \frac{\sin(ql) \sin(qm)}{-(\omega + i\epsilon)^2 + \Omega_q^2}, \\ \text{where } \Omega_q^2 &= \frac{2k_L}{m_L} [1 - \cos(q)].\end{aligned}$$

We need the $(1, 1)^{\text{th}}$ element and the above integral gives $[\mathbf{g}_L^{0+}]_{1,1} = e^{iq}/k_L$, where q is to be obtained from $\omega^2 = (2k_L/m_L)(1 - \cos q)$. For the general case $k_0 \neq k_L$, the Green's function can be calculated as follows. We write $\mathbf{K}_L = \mathbf{K}_L^0 + \Delta\mathbf{K}_L$ where $\Delta\mathbf{K}_L$ is a perturbation matrix whose the only non-zero element is $\Delta\mathbf{K}_{11} = k_0 - k_L$. From the definition of the Green's function $\mathbf{g}_L^+ = [-\mathbf{M}_L(\omega + i\epsilon)^2 + \mathbf{K}_L^0 + \Delta\mathbf{K}_L]^{-1}$ we get

$$\mathbf{g}_L^+ + \mathbf{g}_L^{0+} \Delta\mathbf{K}_L \mathbf{g}_L^+ = \mathbf{g}_L^{0+}. \quad (15)$$

Taking the $(1, 1)^{\text{th}}$ element of the above equation gives

$$[\mathbf{g}_L^+]_{1,1} = \frac{[\mathbf{g}_L^{0+}]_{11}}{1 + [\mathbf{g}_L^{0+}]_{11} [\Delta\mathbf{K}_L]_{11}} = \frac{e^{iq}}{k_L + (k_0 - k_L)e^{iq}}, \quad (16)$$

and similarly

$$[\mathbf{g}_R^+]_{1,1} = \frac{e^{iq'}}{k_R + (k_N - k_R)e^{iq'}}. \quad (17)$$

Using the definitions given earlier we derive the following expressions:

$$\begin{aligned} \Sigma_L^+ &= \frac{k_0^2 e^{iq}}{k_L + (k_0 - k_L)e^{iq}}, & \Sigma_R^+ &= \frac{k_N^2 e^{iq'}}{k_R + (k_N - k_R)e^{iq'}}, \\ \Gamma_L &= -\frac{k_0^2 k_L \sin(q)}{|k_0 - k_L + k_L e^{-iq}|^2}, & \Gamma_R &= -\frac{k_N^2 k_R \sin(q')}{|k_N - k_R + k_R e^{-iq'}|^2}, \end{aligned} \quad (18)$$

where q, q' are respectively obtained from the relations $\omega^2 = (2k_L/m_L)(1 - \cos q) = (2k_R/m_R)(1 - \cos q')$ and Γ_L, Γ_R are non-zero only when both q, q' are real. Plugging in the expressions of Σ_L^+ and Σ_R^+ in Eq. (14), we obtain from Eq. (9)

$$\mathbf{G}_{1,N}^+ = \frac{1}{\begin{bmatrix} 1 & -\frac{k_0^2 e^{iq}}{k_L + (k_0 - k_L)e^{iq}} \end{bmatrix} \hat{T} \begin{bmatrix} k_N & 0 \\ 0 & 1/k_N \end{bmatrix} \begin{bmatrix} 1 \\ \frac{k_N^2 e^{iq'}}{k_R + (k_N - k_R)e^{iq'}} \end{bmatrix}}. \quad (19)$$

III. SCATTERING STATES AND TRANSMISSION COEFFICIENT

For our model the equations of motion correspond to the discrete wave equation for which we can construct scattering wave solutions. We will now construct solutions that correspond to plane waves incident on the system from the reservoirs. From these solutions we will obtain the transmission coefficient. In the following we will only consider the “right-moving states” which correspond to waves that are incident from the left reservoir. The “left-moving states” can be similarly obtained.

Let us consider a chain described by the Hamiltonian of Eq. (2) with an infinite number of particles in both the reservoirs. The particle displacements in the chain satisfy the equations of motion

$$m_l \ddot{x}_l = -(k_{l-1} + k_l) x_l + k_{l-1} x_{l-1} + k_l x_{l+1} , \quad (20)$$

where $l = 1, \dots, N$ refers to particles of the system, $l \leq 0$ refers to particles of the left reservoir (*i.e* $\alpha \geq 1$, as in the notation of Eq. 2), and $l \geq N + 1$ refers to particles in the right reservoir (*i.e* $\alpha' \geq 1$). We note that these equations are valid both for the quantum representation, where the variables are Heisenberg operators, and also for the classical case. Corresponding to the above equations let us construct classical wave solutions ψ_l satisfying the equations

$$m_l \ddot{\psi}_l = -(k_{l-1} + k_l) \psi_l + k_{l-1} \psi_{l-1} + k_l \psi_{l+1} . \quad (21)$$

In the left and right reservoirs these equations take the form of the discrete wave equations

$$\begin{aligned} \ddot{\psi}_\alpha &= (k_L/m_L)(\psi_{\alpha+1} - 2\psi_\alpha + \psi_{\alpha-1}) \quad \text{for } \alpha > 1 , \\ \ddot{\psi}_{\alpha'} &= (k_R/m_R)(\psi_{\alpha'+1} - 2\psi_{\alpha'} + \psi_{\alpha'-1}) \quad \text{for } \alpha' > 1 . \end{aligned}$$

These have the following plane-wave solutions,

$$\psi_\alpha(q) = \frac{1}{(2\pi m_L)^{1/2}} e^{-i\omega t} (e^{-iq\alpha} + r e^{iq\alpha}) \quad \text{for } \alpha \geq 1 , \quad (22)$$

$$\psi_{\alpha'}(q') = \frac{1}{(2\pi m_L)^{1/2}} \tau e^{-i\omega t} e^{iq'\alpha'} \quad \text{for } \alpha' \geq 1 , \quad (23)$$

where the wave-vectors $q, q' \in (0, \pi)$ satisfy the dispersion relations

$$\omega^2 = (2k_L/m_L) (1 - \cos q) = (2k_R/m_R)(1 - \cos q') , \quad (24)$$

and the normalization is chosen such that for $\tau = 0$ (*i.e* no transmission) the following condition is satisfied:

$$\int_0^\pi dq m_L \psi_\alpha^*(q) \psi_\nu(q) = \delta_{\alpha,\nu} \quad (25)$$

for any two points α, ν on the left bath. The solution in Eq. (22) corresponds to a plane wave of wave vector q , frequency ω that is incident on the system from the left side, part of this is then reflected with amplitude r , and a part transmitted across the system with

amplitude τ . We shall refer to τ as the transmission coefficient and will now proceed to the calculation of this. As is well-known in quantum mechanics and wave-theory, the required scattering states can be constructed either by direct solution of the equations of motion in Eq. (21) or by the Lippmann-Schwinger scattering theory approach. We now present both these methods.

A. Transmission coefficient from direct solution of the the wave equation

For points on the reservoirs the plane wave solution has the form in Eq. (22). For $0 \leq l \leq N+1$, let us write $\psi_l(q) = s_l e^{-i\omega t}$, $l = 0, \dots, N+1$ where the amplitudes s_l satisfy the equations

$$m_l \omega^2 s_l = (k_{l-1} + k_l) s_l - k_{l-1} s_{l-1} - k_l s_{l+1}, \quad (26)$$

and it is to be understood that $l = 0, l = -1$ refer to $\alpha = 1, \alpha = 2$ respectively while $l = N+1, l = N+2$ refer to $\alpha' = 1, \alpha' = 2$. Hence we get the following recursion relation:

$$\begin{bmatrix} k_{l-1} s_{l-1} \\ s_l \end{bmatrix} = \hat{T}_l \begin{bmatrix} k_l s_l \\ s_{l+1} \end{bmatrix}, \quad (27)$$

where T_l is defined in Eq. (13). Using this recursively gives

$$\begin{bmatrix} k_{-1} s_{-1} \\ s_0 \end{bmatrix} = \hat{T}_0 \hat{T} \hat{T}_{N+1} \begin{bmatrix} k_{N+1} s_{N+1} \\ s_{N+2} \end{bmatrix}. \quad (28)$$

We note that

$$\begin{bmatrix} k_{-1} s_{-1} \\ s_0 \end{bmatrix} = \frac{1}{(2\pi m_L)^{1/2}} \begin{bmatrix} k_L (e^{-2iq} + r e^{2iq}) \\ (e^{-iq} + r e^{iq}) \end{bmatrix}, \quad \begin{bmatrix} k_{N+1} s_{N+1} \\ s_{N+2} \end{bmatrix} = \frac{1}{(2\pi m_L)^{1/2}} \begin{bmatrix} k_R e^{iq'} \\ e^{2iq'} \end{bmatrix} \tau,$$

$$\hat{T}_0 = \begin{bmatrix} k_L + k_0 - m_L \omega^2 & -k_0^2 \\ 1 & 0 \end{bmatrix}, \quad \hat{T}_{N+1} = \begin{bmatrix} k_R + k_N - m_R \omega^2 & -k_R^2 \\ 1 & 0 \end{bmatrix},$$

and hence Eq. (28) gives

$$\hat{T}_0 \hat{T} \hat{T}_{N+1} \begin{pmatrix} k_R e^{iq'} \\ e^{2iq'} \end{pmatrix} \tau = \begin{pmatrix} k_L e^{-2iq} \\ e^{-iq} \end{pmatrix} + \begin{pmatrix} k_L e^{2iq} \\ e^{iq} \end{pmatrix} r. \quad (29)$$

To solve for τ we multiply the above equation by the row vector $(1 \ -k_L e^{iq})$, and this gives

$$\tau = \frac{-2ik_L \sin(q)}{(e^{iq} - k_L e^{2iq}) \hat{T}_0 \hat{T} \hat{T}_{N+1} \begin{pmatrix} k_R e^{iq'} \\ e^{2iq'} \end{pmatrix}} .$$

After some simplifications and using the form of $\mathbf{G}_{1,N}^+$ given in Eq. (19) we obtain:

$$\tau = -\frac{2ik_L \sin(q) k_0 k_N e^{-i(q+q')}}{(k_0 - k_L + k_L e^{-iq})(k_N - k_R + k_R e^{-iq'})} \mathbf{G}_{1,N}^+ . \quad (30)$$

Now using the expressions for Γ_L, Γ_R in Eq. (18) and comparing with the formula in Eq. (7) we immediately see that the energy transmittance $\mathcal{T}(\omega)$ and the transmission coefficient $\tau(\omega)$ are related as

$$\mathcal{T}(\omega) = |\tau(\omega)|^2 \frac{k_R \sin(q')}{k_L \sin(q)} . \quad (31)$$

B. Transmission coefficient from Lippmann-Schwinger scattering approach

The Lippmann-Schwinger scattering theory approach in quantum mechanics starts by breaking up the Hamiltonian of a system into an unperturbed part and a perturbation. One then writes an exact scattering solution of the unperturbed part of the Hamiltonian and then uses this to obtain a solution of the full problem in terms of the perturbation and appropriate Green's functions. Here, using the notation of Eq. (3), we treat $\mathcal{H}_S + \mathcal{H}_L + \mathcal{H}_R$ as the unperturbed Hamiltonian and $\mathcal{H}_{LS} + \mathcal{H}_{RS}$ as the perturbation.

Lippmann Schwinger theory: Let us use the notation $|\psi(q)\rangle$ to denote the state for the wave-function $\psi_l(q)$ satisfying the wave equation

$$\mathbf{M}\omega^2 |\psi(q)\rangle = \mathbf{K} |\psi(q)\rangle , \quad (32)$$

where \mathbf{M} and \mathbf{K} are the mass matrix and force matrix respectively of the full chain (including system and reservoirs). Using the partition of the chain into the reservoir and system parts, these matrices have the following block structures:

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}_S & 0 & 0 \\ 0 & \mathbf{M}_L & 0 \\ 0 & 0 & \mathbf{M}_R \end{bmatrix} , \quad \mathbf{K} = \begin{bmatrix} \mathbf{K}_S & \mathbf{K}_{SL} & \mathbf{K}_{SR} \\ \mathbf{K}_{SL}^T & \mathbf{K}_L & 0 \\ \mathbf{K}_{SR}^T & 0 & \mathbf{K}_R \end{bmatrix} \quad (33)$$

Breaking \mathbf{K} into unperturbed and perturbed parts we have:

$$\mathbf{K} = \mathbf{K}_0 + \mathbf{K}_1$$

$$\text{where} \quad \mathbf{K}_0 = \begin{bmatrix} \mathbf{K}_S & 0 & 0 \\ 0 & \mathbf{K}_L & 0 \\ 0 & 0 & \mathbf{K}_R \end{bmatrix}, \quad \mathbf{K}_1 = \begin{bmatrix} 0 & \mathbf{K}_{SL} & \mathbf{K}_{SR} \\ \mathbf{K}_{SL}^T & 0 & 0 \\ \mathbf{K}_{SR}^T & 0 & 0 \end{bmatrix}. \quad (34)$$

Treating \mathbf{K}_1 as a perturbation we then obtain the following scattering solution of Eq. (32):

$$|\psi\rangle = |\psi^0\rangle - \mathcal{G}^+ \mathbf{K}_1 |\psi^0\rangle,$$

$$\text{where } \mathcal{G}^+ = [-\mathbf{M}(\omega + i\epsilon)^2 + \mathbf{K}]^{-1} \quad (35)$$

is the Green's function for the full chain and $|\psi^0\rangle$ is a scattering solution of the unperturbed system satisfying the equation

$$\mathbf{M}\omega^2 |\psi^0(q)\rangle = \mathbf{K}_0 |\psi^0(q)\rangle. \quad (36)$$

Construction of initial state: Let us first construct the right-moving scattering states. For this we consider the particular initial state $|\psi^0\rangle$ where the left reservoir is in a normal mode with frequency ω while the system and right reservoir degrees of freedom are at rest. Thus we choose $\psi_l^0(q) = 0$ for $l > 0$ and $\psi_l^0(q) = \psi_\alpha^L$ for $l \leq 0$, with $\alpha = 1 - l$ and $\psi_\alpha^L(q)$ satisfying the equation

$$m_L \omega^2 \psi_\alpha^L(q) = \sum_{\beta} [\mathbf{K}_L]_{\alpha,\beta} \psi_\beta^L(q). \quad (37)$$

The form of \mathbf{K}_L can be read from Eq. (4), and we then get

$$m_L \omega^2 \psi_\alpha^L(q) = k_L [2\psi_\alpha^L(q) - \psi_{\alpha+1}^L(q) - \psi_{\alpha-1}^L(q)] + \delta_{\alpha,1}(k_0 - k_L)\psi_1^L(q), \quad \alpha = 1, 2, \dots, \quad (38)$$

with the boundary condition $\psi_0^L(q) = 0$. For $k_0 = k_L$ the normal modes are given by $\psi_\alpha^L(q) = 2i \sin q\alpha / (2\pi m_L)^{1/2}$, where the normalization is chosen such that $\int_0^\pi dq m_L \psi_\alpha^{L*}(q) \psi_\nu^L(q) = \delta_{\alpha,\nu}$. For $k_0 \neq k_L$ we can find the normal modes by treating the last term in Eq. (38) as a perturbation. We will require only $\psi_{\alpha=1}^L(q)$. The Lippmann-Schwinger approach is applied again, giving

$$\psi_{\alpha=1}^L(q) = \frac{2i \sin(q)}{(2\pi m_L)^{1/2}} [1 - (k_0 - k_L) [\mathbf{g}_L^+]_{1,1}] = -\frac{2i \sin q}{(2\pi m_L)^{1/2}} k_L e^{-iq} [\mathbf{g}_L^+]_{1,1}, \quad (39)$$

where the result in Eq. (16) has been used. Note that our choice of ψ_0^L implies an incident wave $e^{iq\alpha}/(2\pi m_L)^{1/2}$.

Scattering state: Since we want to finally find τ , it is sufficient to compute the scattering wave function only on the right reservoir. From Eq. (35) we get

$$\psi_{\alpha'}(q) = -\mathcal{G}_{\alpha',l=1}^+ k_0 \psi_{\alpha=1}^L(q) . \quad (40)$$

We now express the Green's function element $-\mathcal{G}_{\alpha',l=1}^+$ in terms of the Green's function \mathbf{G}^+ defined earlier in Eq. (5). We first write \mathcal{G}^+ in a block-matrix form, with the different blocks representing the system and reservoirs. This matrix satisfies the following relation:

$$\begin{bmatrix} -\mathbf{M}^S(\omega + i\epsilon)^2 + \mathbf{K}_S & \mathbf{K}_{SL} & \mathbf{K}_{SR} \\ \mathbf{K}_{SL}^T & -\mathbf{M}^L(\omega + i\epsilon)^2 + \mathbf{K}_L & 0 \\ \mathbf{K}_{SR}^T & 0 & -\mathbf{M}^R(\omega + i\epsilon)^2 + \mathbf{K}_R \end{bmatrix} \times \begin{bmatrix} \mathbf{G}_S^+ & \mathbf{G}_{SL}^+ & \mathbf{G}_{SR}^+ \\ \mathbf{G}_{LS}^+ & \mathbf{G}_L^+ & \mathbf{G}_{LR}^+ \\ \mathbf{G}_{RS}^+ & \mathbf{G}_{RL}^+ & \mathbf{G}_R^+ \end{bmatrix} = \begin{bmatrix} \mathbf{I} & 0 & 0 \\ 0 & \mathbf{I} & 0 \\ 0 & 0 & \mathbf{I} \end{bmatrix} . \quad (41)$$

From this equation the following relations can be shown to hold [1]:

$$\mathbf{G}_S^+(\omega) = \frac{1}{-\omega^2 \mathbf{M}^S + \mathbf{K}_S - \Sigma_L^+ - \Sigma_R^+} =: \mathbf{G}^+(\omega) , \quad (42)$$

$$\mathbf{G}_{RS}^+ = \mathbf{g}_R^+ \mathbf{K}_{SR} \mathbf{G}^+ . \quad (43)$$

This then gives us

$$\mathcal{G}_{\alpha',l=1}^+ = [\mathbf{G}_{RS}^+]_{\alpha',l=1} = [\mathbf{g}_R^+]_{\alpha',1} k_N \mathbf{G}_{N,1}^+ . \quad (44)$$

Using Eqs. (39,44) in Eq. (40) we finally get:

$$\psi_{\alpha'}(q') = 2ik_0 k_N k_L \sin q e^{-iq} [\mathbf{g}_L^+]_{1,1} [\mathbf{g}_R^+]_{\alpha',1} \mathbf{G}_{1,N}^+ / (2\pi m_L)^{1/2} . \quad (45)$$

Now taking the $(\alpha', 1)^{\text{th}}$ element of Eq. (15), with L replaced by R , and using Eq. (17) we get

$$[\mathbf{g}_R^+]_{\alpha',1} = \frac{e^{iq'\alpha'}}{k_R + (k_N - k_R)e^{iq'}} . \quad (46)$$

Using the explicit form of $[\mathbf{g}_L^+]_{1,1}$ from Eq. (16) we finally arrive at the expected form of the transmitted wave function in the right reservoir

$$\psi_{\alpha'}(q') = \tau e^{iq'\alpha'} / (2\pi m_L)^{1/2}$$

with τ precisely given by the same expression Eq. (30) obtained in the previous sub-section by the direct solution of the wave equation.

IV. EXPRESSION FOR THE ENERGY CURRENT IN EACH MODE AND A DERIVATION OF THE LANDAUER FORMULA

We now use the definition of the heat current operator and show how it can be used to express the current contribution of each of the modes in terms of the transmission coefficient and hence the energy transmittance. This will lead us to a derivation of the Landauer formula. In the steady state the current is constant everywhere and we will evaluate it on the right reservoir. Between sites α' and $\alpha' + 1$ the left-right current is given by the expectation value [2] $\hat{j}_L = \langle \frac{1}{2}k_R(v_{\alpha'} + v_{\alpha'+1})(x_{\alpha'} - x_{\alpha'+1}) \rangle$ where we compute the average using the q^{th} right-moving state obtained in the previous section. It is easiest to obtain this using second-quantized notation. The set of right moving and left moving states form a complete set. Denoting the left-movers by $\psi_{\alpha'}(q)$ with $q \in (-\pi, 0)$ we note that they satisfy the completeness relation $\int_{-\pi}^{\pi} dq (m_{\alpha'})^{1/2} (m_{\nu'})^{1/2} \psi_{\alpha'}^*(q) \psi_{\nu'}(q) = \delta_{\alpha', \nu'}$. The displacement and velocity operators at the lattice sites of the right bath can be expressed in terms of the creation and annihilation operators $a_{q'}, a_{q'}^\dagger$ as

$$\begin{aligned} x_{\alpha'} &= \int_{-\pi}^{\pi} dq \left(\frac{\hbar}{2\omega_q} \right)^{\frac{1}{2}} (a_q \psi_{\alpha'}(q) + a_q^\dagger \psi_{\alpha'}^*(q)) , \\ v_{\alpha'} &= -i \int_{-\pi}^{\pi} dq \left(\frac{\hbar\omega_q}{2} \right)^{\frac{1}{2}} (a_q \psi_{\alpha'}(q) - a_q^\dagger \psi_{\alpha'}^*(q)) . \end{aligned}$$

The operators $a_{q_1}, a_{q_2}^\dagger$ satisfy the commutation relations $[a_{q_1}, a_{q_2}^\dagger] = \delta(q_1 - q_2)$ and, using the completeness relation, it can be verified that this ensures the usual commutation relations for the position and momentum operators. Using the above we get for the expectation value of the current for a right moving state:

$$\begin{aligned} J_{LR}(q) &= i\hbar k_R (\langle a_q^\dagger a_q \rangle + \frac{1}{2}) [\psi_{\alpha'+1}^*(q) \psi_{\alpha'}(q) - \psi_{\alpha'+1}(q) \psi_{\alpha'}^*(q)] \\ &= \frac{\hbar k_R \sin(q')}{\pi m_L} |\tau|^2 [f(\omega_q, T_L) + \frac{1}{2}] , \end{aligned} \tag{47}$$

where in the last step we have used the form $\psi_{\alpha'}(q) = \tau e^{i\alpha'q'} / (2\pi m_L)^{1/2}$, and the initial occupation probability of the state q is given by the left bath thermal distribution $\langle a_q^\dagger a_q \rangle = [e^{\hbar\omega_q/k_B T_L} - 1]^{-1} = f(\omega, T_L)$. The total current transmitted from the left bath to the right

bath, is obtained by integrating over all q . After making a change of variables from q to $\omega = 2(k_L/m_L)^{1/2}\sqrt{1 - \cos(q)}$ we get

$$\begin{aligned}
J_{LR} &= \int_0^\pi dq J_{LR}(q) \\
&= \frac{1}{\pi} \int_0^{2(k_L/m_L)^{1/2}} d\omega \hbar\omega \frac{k_R \sin(q')}{k_L \sin q} |\tau|^2 [f(\omega, T_L) + \frac{1}{2}] \\
&= \frac{1}{\pi} \int_0^{2(k_L/m_L)^{1/2}} d\omega \hbar\omega \mathcal{T}(\omega) [f(\omega, T_L) + \frac{1}{2}] ,
\end{aligned} \tag{48}$$

where in the last step we used Eq. (31). From symmetry, the current flowing from the right bath to the left bath will be given by

$$J_{RL} = \frac{1}{\pi} \int_0^{2(k_R/m_R)^{1/2}} d\omega \hbar\omega \mathcal{T}(\omega) [f(\omega, T_R) + \frac{1}{2}] .$$

Hence finally we get for the net current:

$$J = \frac{1}{\pi} \int_0^{\omega_m} d\omega \hbar\omega \mathcal{T}(\omega) [f(\omega, T_L) - f(\omega, T_R)] , \tag{49}$$

where $\omega_m = \min[2(k_L/m_L)^{1/2}, 2(k_R/m_R)^{1/2}]$. Observing that \mathcal{T} is a symmetric function of ω and vanishes outside the range $\omega \in (0, \omega_m)$, we can see that Eq. (49) is equivalent to the Landauer formula Eq. (1).

V. DISCUSSION

In summary we have studied heat conduction across a 1D quantum-mechanical harmonic chain, with arbitrary distribution of masses and inter-particle spring constants, that is connected to two other ordered 1D harmonic crystals which have different mass densities and elastic constants. For this model we use two different approaches to demonstrate the relation $\mathcal{T}(\omega) = (k_R \sin q') |\tau(\omega)|^2 / (k_L \sin q)$ between the energy transmittance $\mathcal{T}(\omega)$, which occurs in the Landauer formula for heat current, and the transmission coefficient $\tau(\omega)$ related to passage of plane waves across the system. In the first approach we use the fact that the Green's function occurring in the expression for \mathcal{T} has a simple representation in terms of product of 2×2 matrices. The plane wave solutions are then obtained by directly solving the equations of motion and a representation of τ is obtained, again in terms of the product of matrices. The connection between \mathcal{T} and τ is then directly obtained. This approach can

be extended to the case of regular lattices using, for example, the techniques used in [19] for the representation of the Green's functions using matrix products.

In the second approach it is not necessary to find the explicit form of the Green's function. One notes that the required plane wave scattering states can be obtained by using the Lippmann-Schwinger approach to evolve initial states which are eigenmodes of either one of the reservoirs and are initially localized within the reservoirs. The Lippmann-Schwinger approach then directly gives τ in terms of the Green's function. This second approach is more powerful since it can be used for arbitrary harmonic structures where it is not possible to think of simple plane wave scattering states. This approach tells us that we need to construct scattering states by evolving the eigenmodes of the two isolated reservoirs. Indeed this is what the NEGF approach does in effect and our explicit calculations for a simple but representative model clarifies the picture. Our exact calculations also illustrate some of the subtle points involved, such as the correct computation of the self-energies Σ_L^+, Σ_R^+ for inhomogeneous chains, appropriate normalizations of normal-modes and the choice of initial states.

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